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ME469: Common Discretization Approaches: Edge-based, Vertex-Centred (EBVC), and Cell-Centred (CC)

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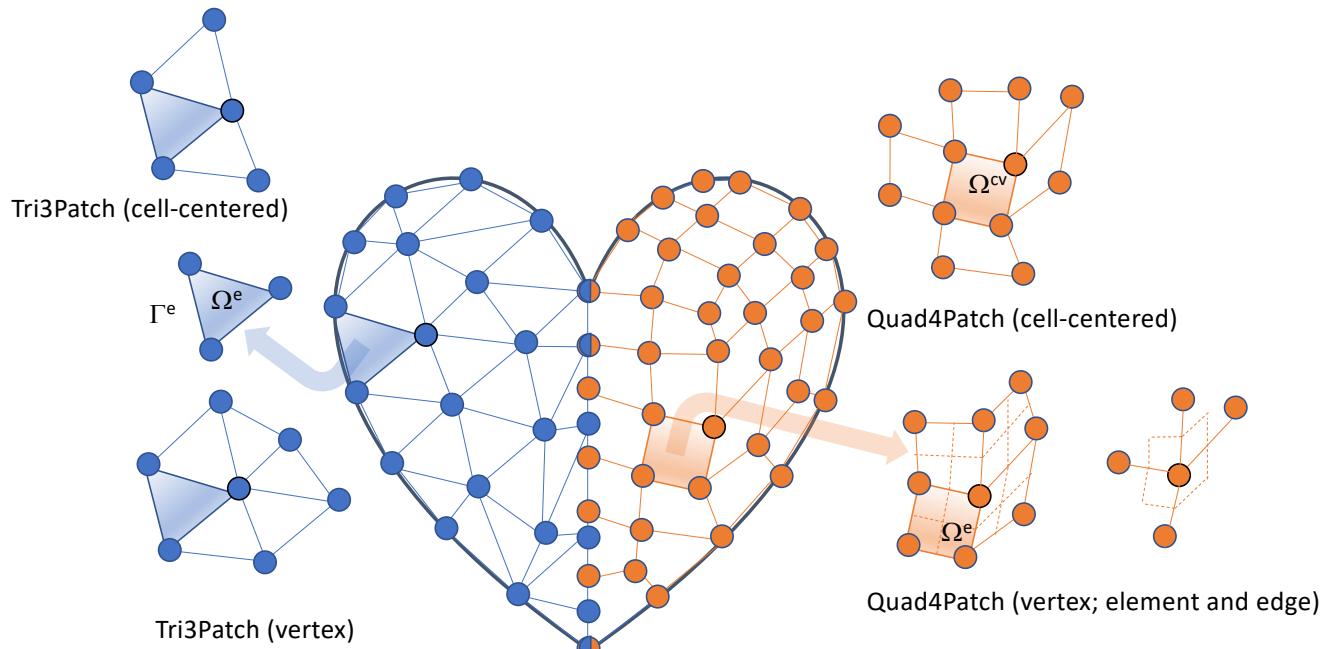
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Review of Discretization Options

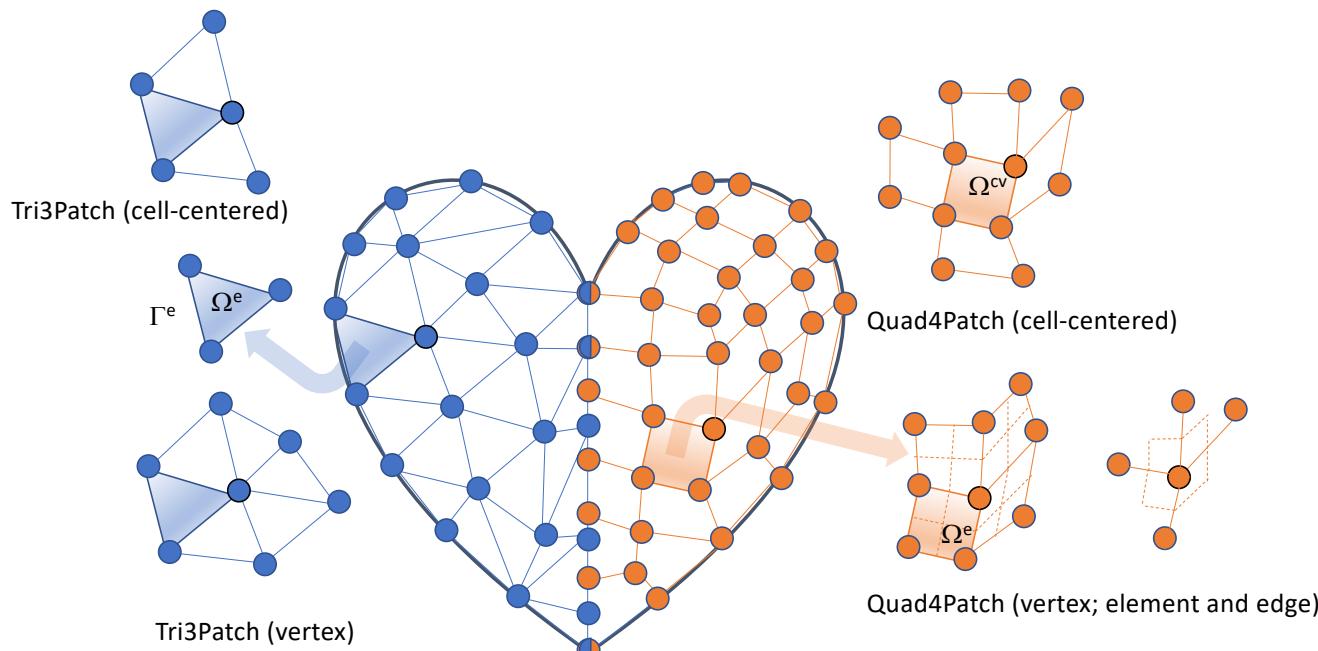
- Degree-of-freedom (DOF) for:
 - Cell-centered: Stencil is based on a element:face:element
 - DOFs at vertices of elements, or “nodes”, element:node (CVFEM, FEM), edge:node (EBVC)



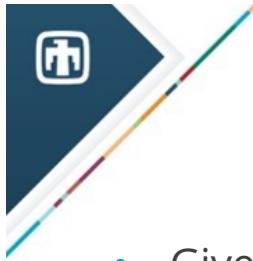


Review of Discretization Options: New, a nodal-basis...

- Degree-of-freedom (DOF) for:
 - Cell-centered: Stencil is based on a element:face:element
 - DOFs at vertices of elements, or “nodes”, element:node (CVFEM, FEM), edge:node (EBVC)



- Definition of an interpolation function:
$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$
- N_n^{ip} is the Lagrange function associated with node n
- ϕ_n is the value of the DOF at node n
- The nodal basis functions obey equipartition of unity and satisfy, $N_n^{x_j} = \delta_{nj}$



Fundamentals of Discretization: Surface vs Volume Integrations

- Given a partial differential equation (PDE) and associated volumetric form:

$$\int \frac{\partial F_j}{\partial x_j} dV = \int S dV$$

- Applying Gauss Divergence provides the standard finite volume form for fluxes in surface integral form:

$$\int \frac{\partial F_j}{\partial x_j} dV = \int F_j n_j dS \quad \longrightarrow \quad \int F_j n_j dS = \int S dV$$

- We can also multiply PDE by an arbitrary test function, w , and integrate over a volume,

$$\int w \frac{\partial F_j}{\partial x_j} dV = \int w S dV$$

$$\int \frac{\partial w}{\partial x_j} F_j dV - \int w F_j dS = \int w S dV$$

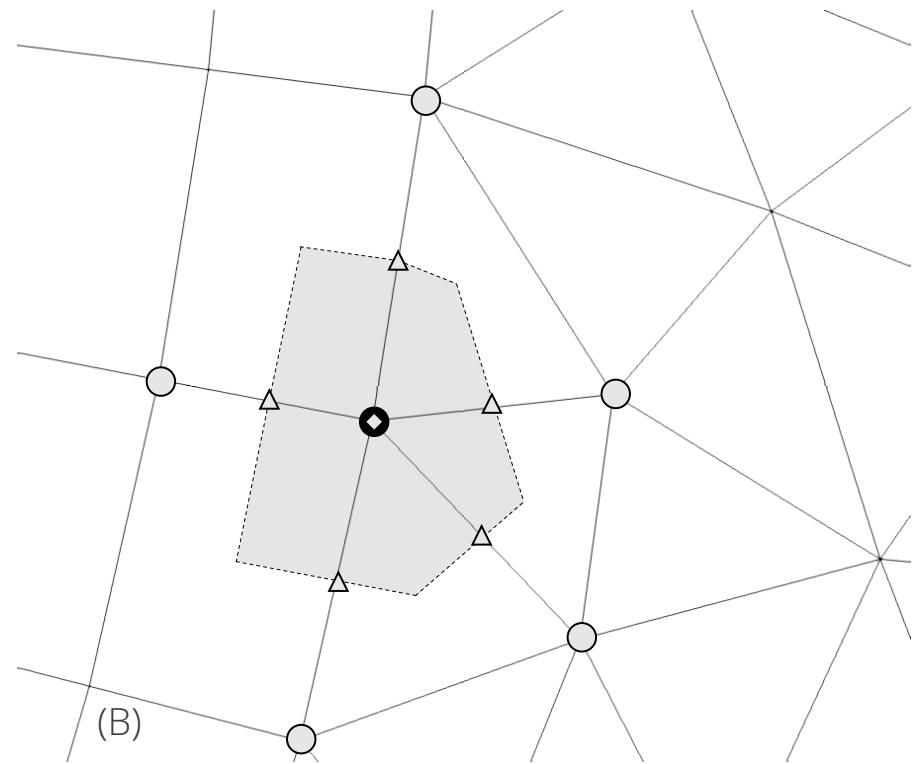
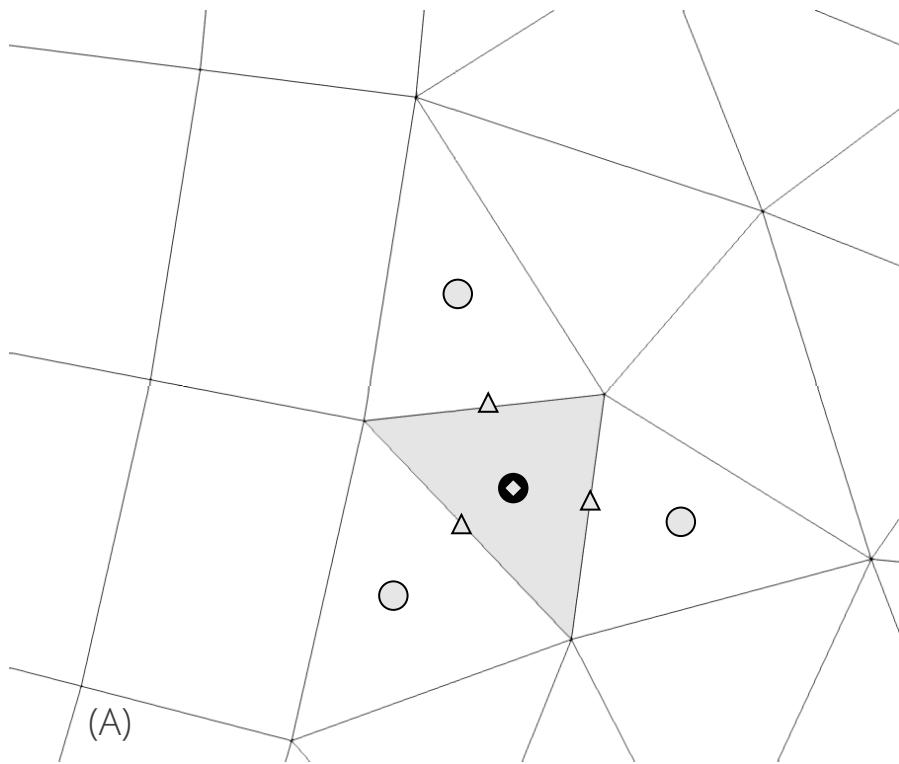
Next, integrate by parts and apply Gauss-Divergence. Note, that test function must be differentiable – shown here, at least once..

$$\frac{\partial w F_j}{\partial x_j} = w \frac{\partial F_j}{\partial x_j} + \frac{\partial w}{\partial x_j} F_j$$



Cell-Centered (CC) and Edge-Based Vertex-Centred (EBVC): Each are generally a two-state scheme, Left (L) and Right(R)

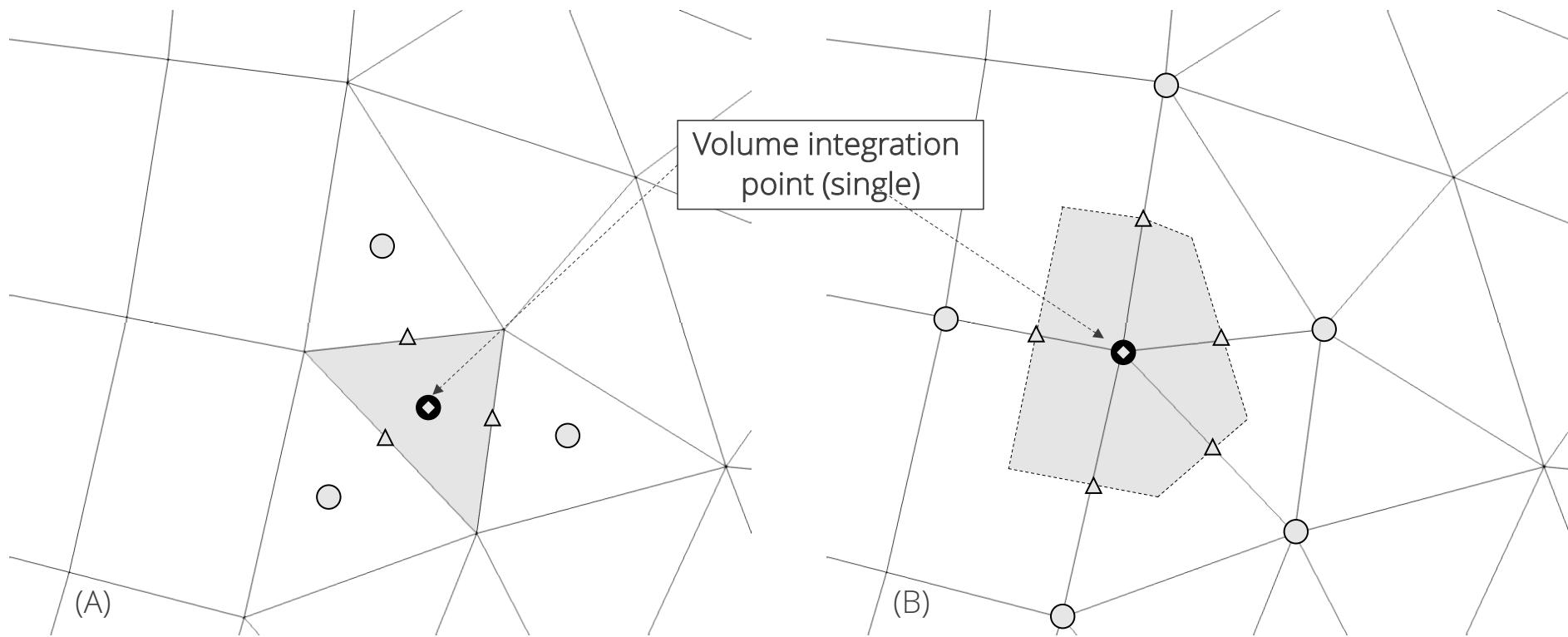
- CC (A) and EBVC (B) – As shown below, each have a set of common features
 - Class Discussion: What are the common features?





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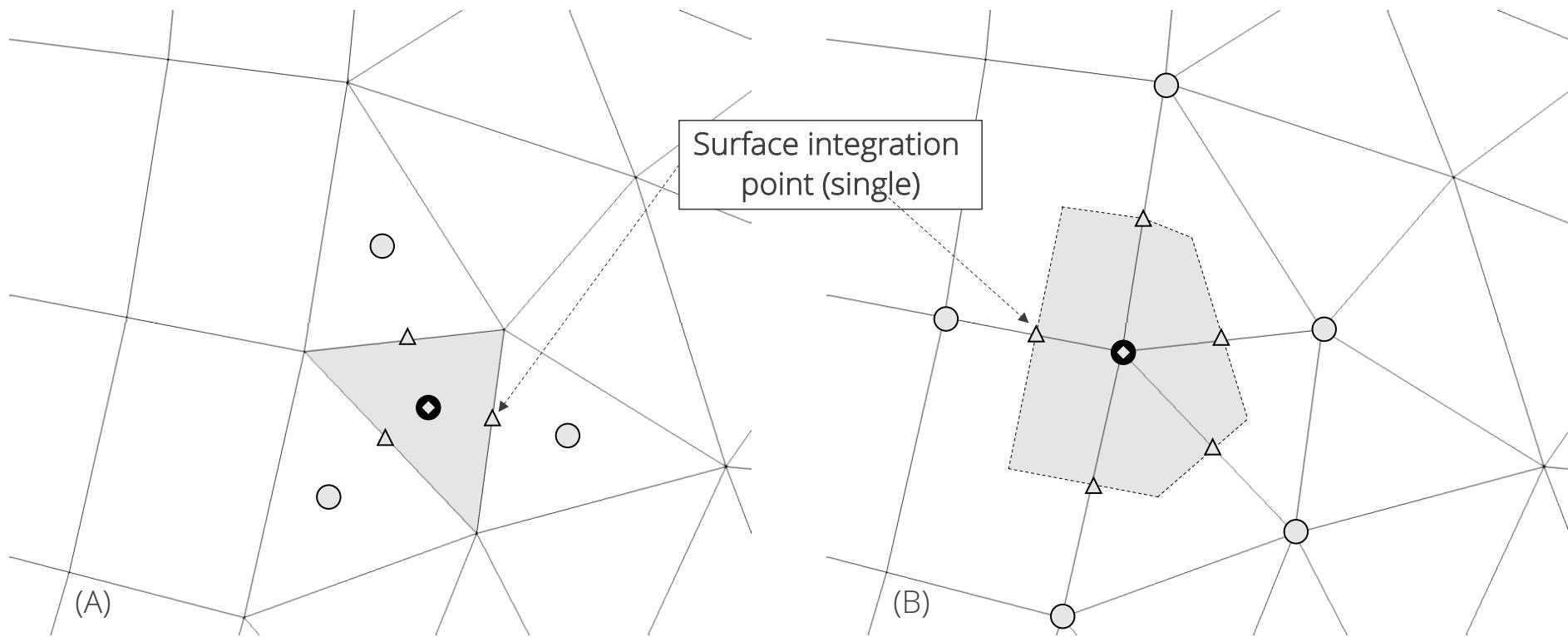
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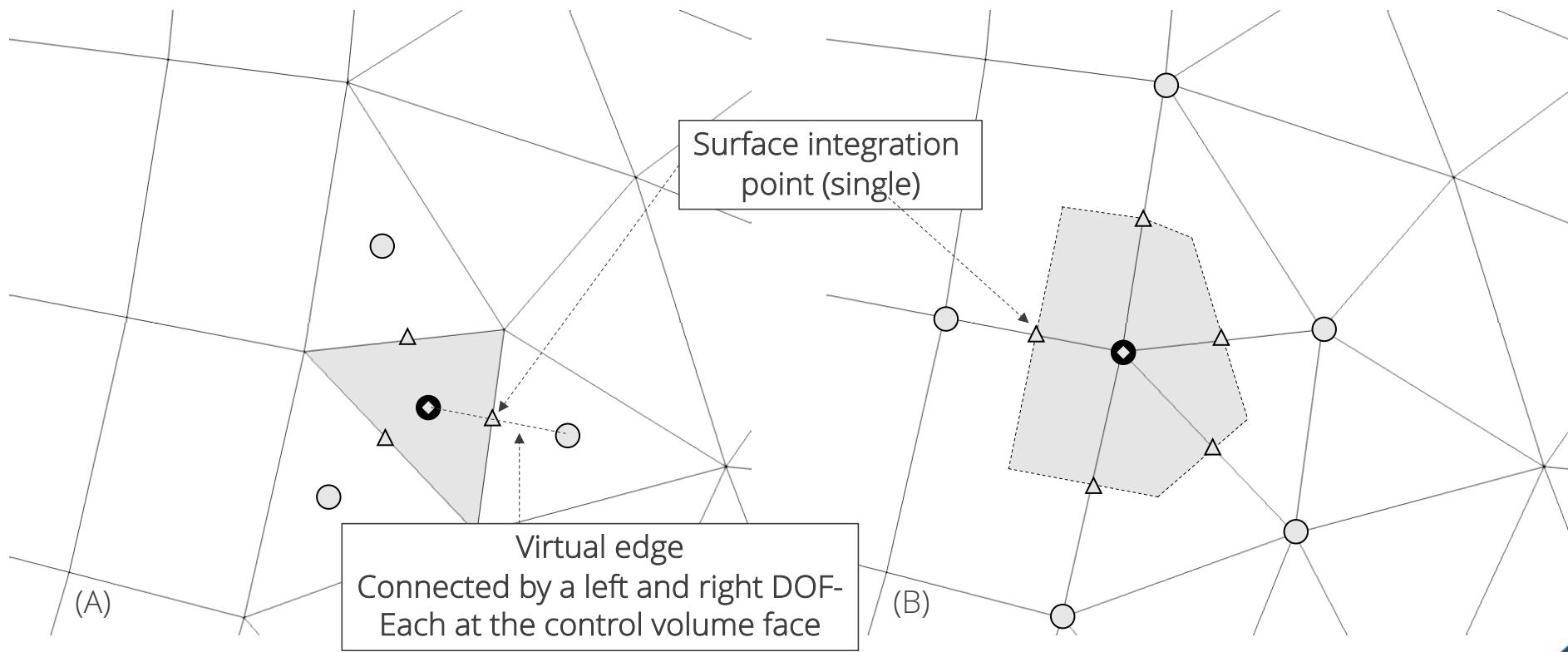
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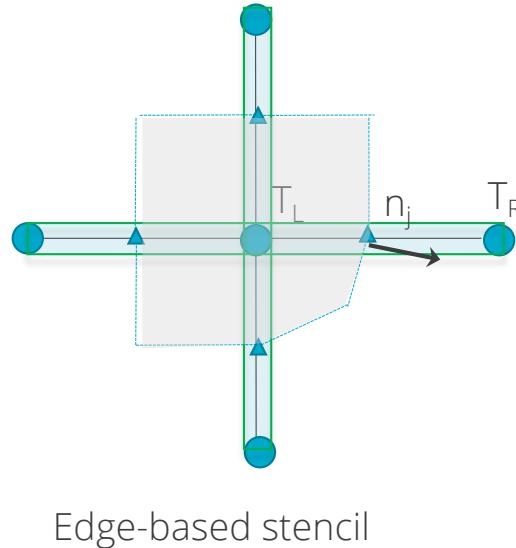
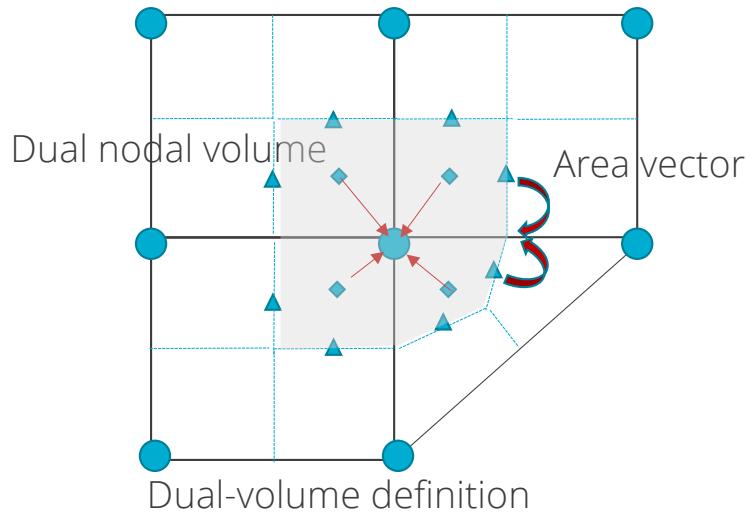
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The Control Volume for EBVC is Defined by the **Dual-Volume**

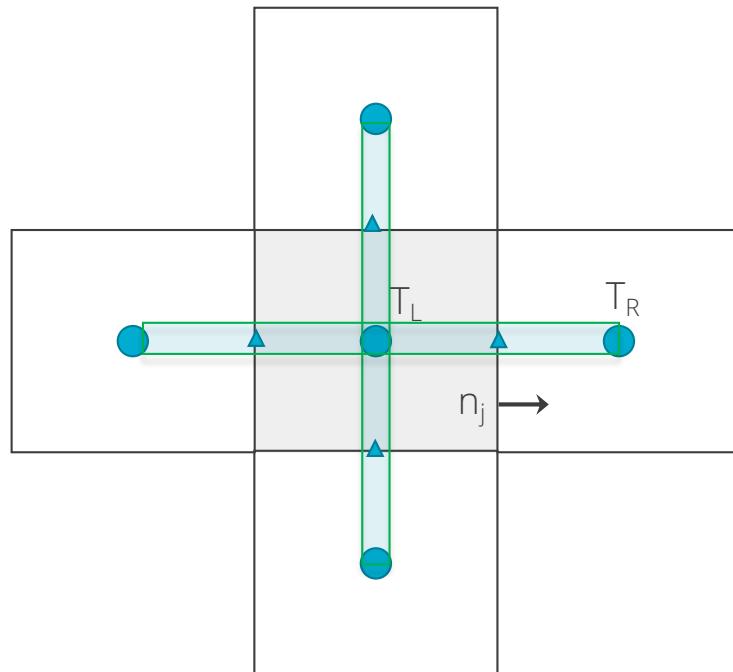
- All primitives are collocated at the vertices of the elements with equal-order interpolation
- A dual mesh is constructed to obtain flux and volume quadrature locations
- Classic two-state, “L” and “R” approach provides spatially second-order accuracy
- Iterate **Nodes** for volume-based contributions
- Iterate **Edges** for surface-based contributions





The Control Volume for CC is Defined by the ***Element Volume***

- All primitives are collocated at the cell-center of the element with equal-order interpolation
- Classic two-state, “L” and “R” approach provides spatially second-order accuracy
- Iterate ***Elements*** for volume-based contributions
- Iterate ***Virtual-Edges*** or ***Control Volume Faces*** for surface-based contributions





One-Dimensional Example of a Non-Uniform Mesh

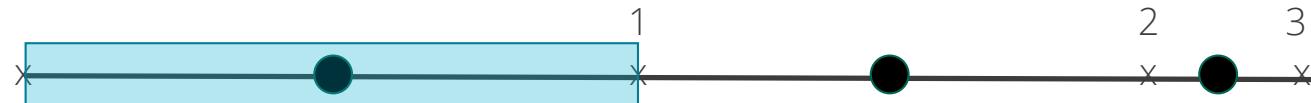
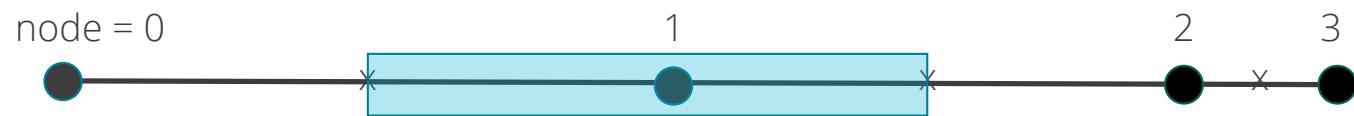
- The nodes of the mesh need-not be equally spaced





Control Volumes for CC and EBVC

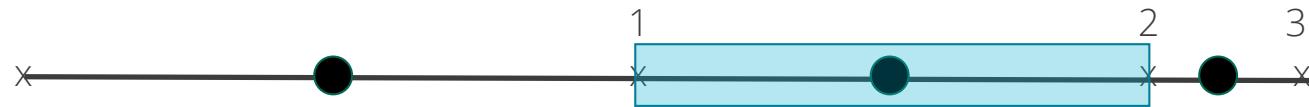
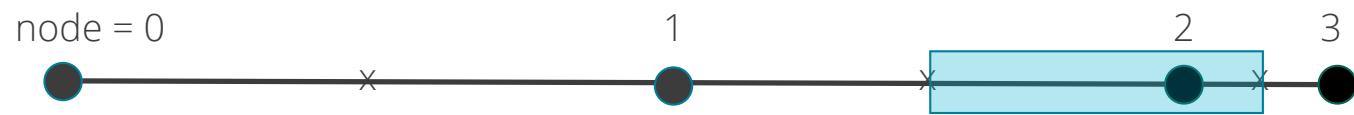
- Note: Switched depiction of node (or vertex) to the cell-centered location





Control Volumes for CC and EBVC

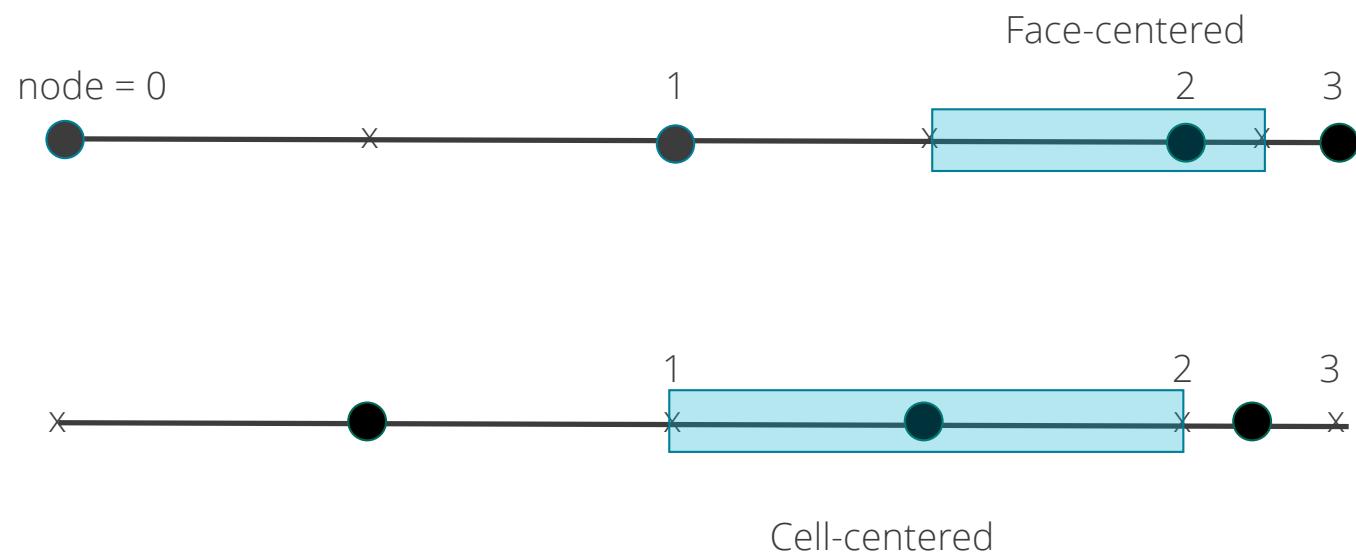
- Note: Switched depiction of node (or vertex) to the cell-centered location





Control Volumes for CC and EBVC

- Face-centered vs Cell-Centered





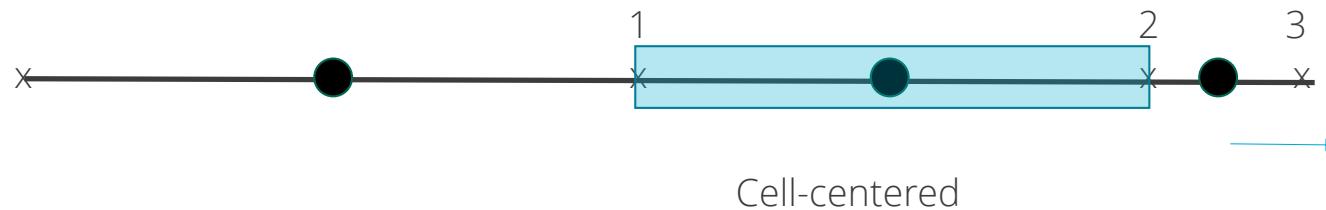
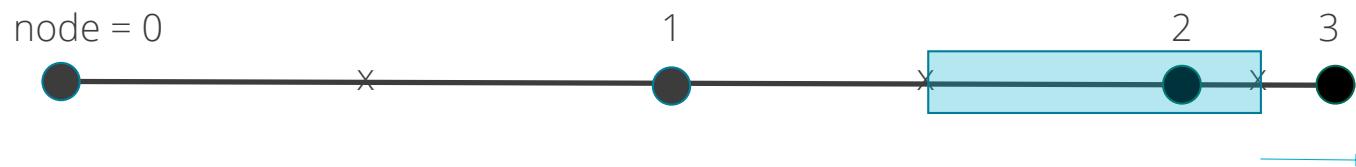
Basis Function Re-Visited

- Define an isoparametric base element that varies from -1:+1, with integration point at the location ξ :

$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

$$N_1 = \frac{(1 - \xi)}{2}$$

$$N_2 = \frac{(1 + \xi)}{2}$$





Basis Function Re-Visited

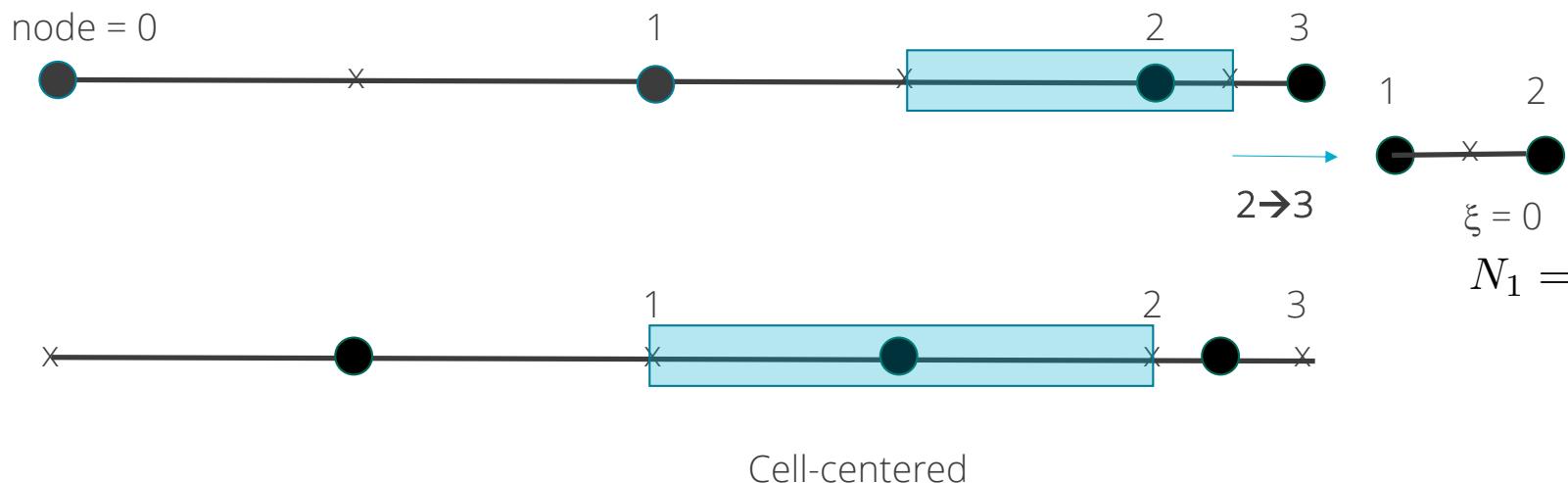
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$$N_2 = \frac{(1 + \xi)}{2}$$



$$N_1 = N_2 = \frac{1}{2}$$



Basis Function Re-Visited

- Define an isoparametric base element that varies from -1:+1, with integration point at the location ξ :

$$\phi_{ip} = \sum_n N_n^{ip} \phi_n$$

$$N_1 = \frac{(1 - \xi)}{2}$$

$$N_2 = \frac{(1 + \xi)}{2}$$

node = 0



*

1

*

*

Face-centered

2

3

1

2

$2 \rightarrow 3$

$\xi = 0$

$$N_1 = N_2 = \frac{1}{2}$$

*

*

1

*

2

3

Cell-centered

$1 \rightarrow 2$

$\xi = 1/2$

$$N_1 = \frac{1}{4}; N_2 = \frac{3}{4}$$



Other Examples of a Basis (This will become important for the element-based schemes)

Linear (Quad4)

$$N_1 = \frac{1}{4}(1 - \xi)(1 - \eta)$$

$$N_2 = \frac{1}{4}(1 + \xi)(1 - \eta)$$

$$N_3 = \frac{1}{4}(1 + \xi)(1 + \eta)$$

$$N_4 = \frac{1}{4}(1 - \xi)(1 + \eta)$$

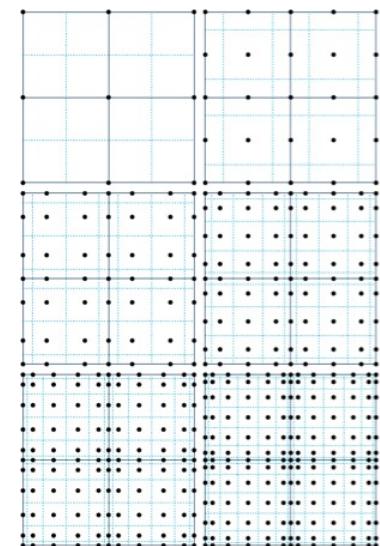
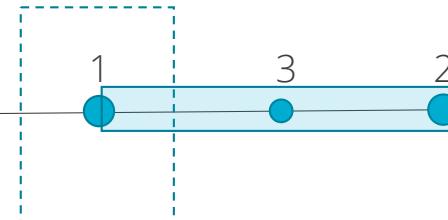
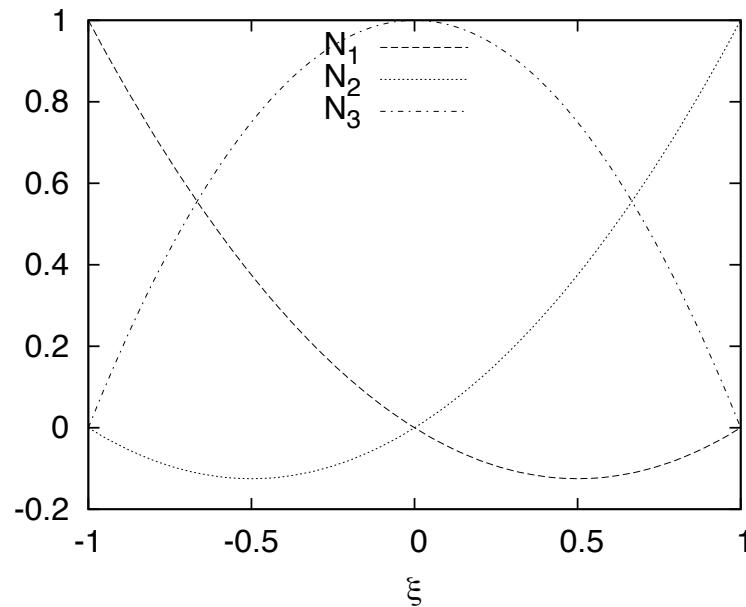
Quadratic (Bar3)

$$N_1 = \frac{-\xi(1 - \xi)}{2}$$

$$N_2 = \frac{\xi(1 + \xi)}{2}$$

$$N_3 = (1 - \xi)(1 + \xi)$$

$\widehat{\xi}$



Two-dimensional promotion



Simple One-D Diffusion Example

Let us introduce (briefly) the Method of Manufactured Solutions (MMS)

- Consider a simple diffusion equation:

$$\frac{d^2\phi}{dx^2} = 0$$

with a presumed, or manufactured solution:

$$\phi^{MMS}(x) = x^2$$

$$\frac{d^2\phi^{MMS}}{dx^2} = S^{MMS} = 2$$

Gauss-Divergence

$$\int \frac{d^2\phi^h}{dx^2} dV = \int S^{MMS} dV \quad \int \frac{d\phi^h}{dx} dS = \int S^{MMS} dV$$

Discrete flux-based form at the sub-control volume surface (scs) and sub-control volume IP:

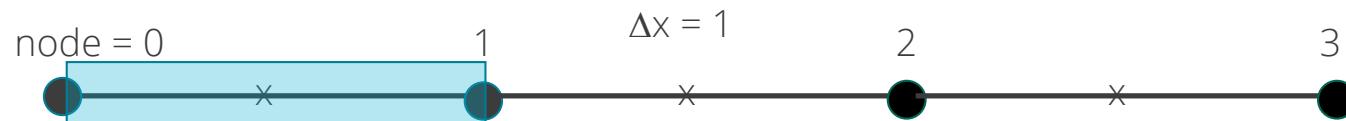
With error: $\epsilon = \phi^{MMS} - \phi^h$

$$\sum_{scsIP} \frac{d\phi^h}{dx} A_{scsIP} = \sum_{scvIP} S^{MMS} V_{scvIP}$$



Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: $+= L$ and $-= R$
 (note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_1^h - \phi_0^h}{\Delta x} + C_0(\Delta x) + \dots$$

$$LHS_0+ = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

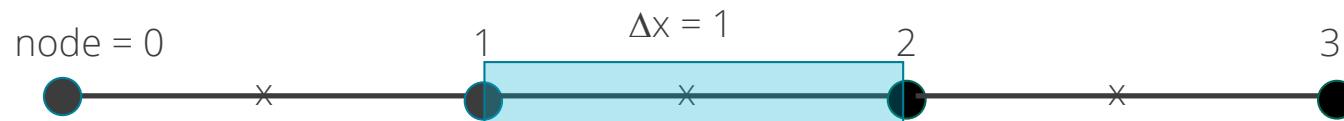
$$LHS_1- = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

Edge 1



Simple One-D MMS Example; Edge-based Assemble of Diffusion

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Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: $+= L$ and $-= R$
 (note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_2^h - \phi_1^h}{\Delta x} + C_0(\Delta x) + \dots$$

$$LHS_1+ = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

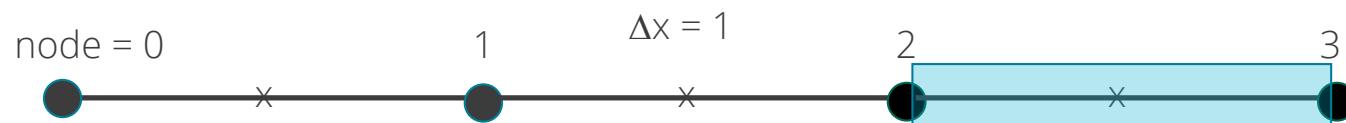
$$LHS_2- = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

Edge 2



Simple One-D MMS Example; Edge-based Assemble of Diffusion

We will use a linear basis and solve this system over a small patch of linear bar elements



Recall, simplified equation with RHS from source term already provided

$$\sum_{scsIP} \frac{d\phi^h}{dx}_{scsIP} = \sum_{scvIP} S^{MMS} \frac{\Delta x}{2}$$

Iterate elements with a simple left-hand side rule: += L and -=R

(note implicit conservation statement)

$$\frac{d\phi^h}{dx}_{scsIP} = \frac{\phi_3^h - \phi_2^h}{\Delta x} + C_0(\Delta x) + \dots$$

$$LHS_{2+} = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$LHS_{3-} = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

Edge 3



Simple One-D MMS Example; Collect all of the terms

$$LHS_0+ = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1- = \frac{\phi_1^h - \phi_0^h}{\Delta x}$$

$$LHS_1+ = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2- = \frac{\phi_2^h - \phi_1^h}{\Delta x}$$

$$LHS_2+ = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$LHS_3- = \frac{\phi_3^h - \phi_2^h}{\Delta x}$$

$$A = \frac{1}{\Delta x} \begin{bmatrix} -1 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & +1 & -1 \end{bmatrix}$$

Fully assembled matrix

$$\frac{1}{\Delta x} \begin{bmatrix} -1 & +1 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & +1 & -1 \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 2 \\ 2 \\ 2 \end{bmatrix}$$

Fully assembled system

$$\frac{1}{\Delta x} \begin{bmatrix} +1 & 0 & 0 & 0 \\ +1 & -2 & +1 & 0 \\ 0 & +1 & -2 & 1 \\ 0 & 0 & 0 & +1 \end{bmatrix} \begin{bmatrix} \phi_0 \\ \phi_1 \\ \phi_2 \\ \phi_3 \end{bmatrix} = \begin{bmatrix} 0 \\ 2 \\ 2 \\ 9 \end{bmatrix}$$

Correct for BCs

$$\phi^h = \begin{bmatrix} 0 \\ 1 \\ 4 \\ 9 \end{bmatrix}$$

Solution is exact.... Linear basis exactly captures a quadratic solution



Model Passive Scalar Transport: Introducing the Test Function, w

- Time/Src/Advection/Diffusion equation for scalar ϕ

$$\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\rho D \frac{\partial \phi}{\partial x_j} \right) = S^\phi$$

Under the assumption, $\rho D = \frac{\mu}{Sc}$ yields: $\frac{\partial \rho\phi}{\partial t} + \frac{\partial \rho u_j \phi}{\partial x_j} - \frac{\partial}{\partial x_j} \left(\frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) = S^\phi$

We can also integrate this PDE over the volume, while introducing a test function, w

$$\int w \left(\frac{\partial \rho\phi}{\partial t} + \frac{\partial}{\partial x_j} \left(\rho u_j \phi - \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) - S^\phi \right) dV = \int w R(\phi) dV$$

- The above is the so-called weak-form of the original (strong form) partial differential equation
- The elegant concept of a weighted residual statement is to seek a weak solution such that the residual is orthogonal to a selected space of weight functions



Model Passive Scalar Transport: Integration-by-Parts

- Recall, integration-by-parts, for example,

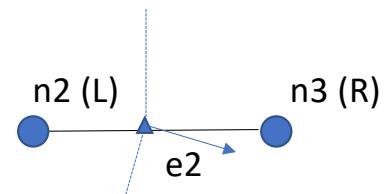
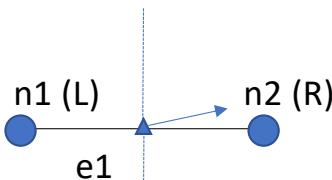
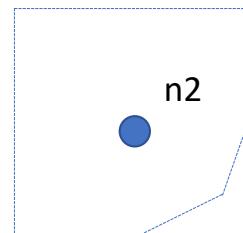
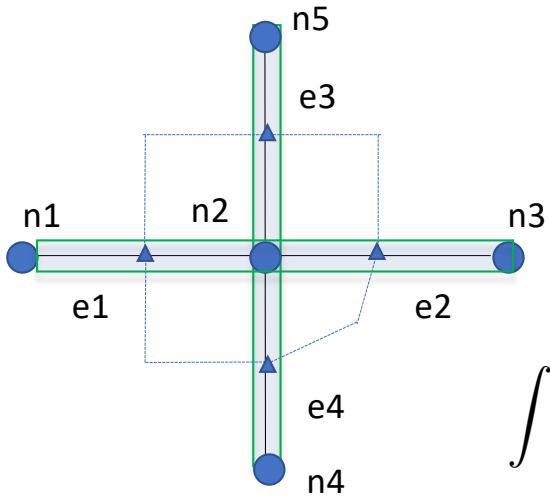
$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV = - \int \rho u_j \phi \frac{\partial w}{\partial x_j} dV + \int w \rho u_j \phi n_j dS$$

- Note, that w must be differentiable at least once
- Under the special designation of w to be a piecewise constant, or Heaviside function, the gradient of this is a (negative) Diract-delta function
- A key property of this function is that the gradient of the piece-wise constant test function is a distribution of delta functions on the sub-control volume surface yielding,
$$\int \left(\frac{\partial \rho \phi}{\partial t} - S^\phi \right) dV + \int \left(\rho u_j \phi - \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} \right) n_j dS = 0$$
- Recall, we could have arrived at this form by simply usage of Gauss-Divergence, however, this formality allows us to view a finite volume scheme as a Petrov-Galerkin scheme, i.e., the underlying basis differs from the test function

Deep Dive on EBVC: Node and Edge-loops

EBVC is a discretization scheme that:

- Uses a piecewise-constant test function
- Is a two-state flux approach, with a face-centered arrangement
- Iterates over locally-owned nodes for Time/Source/etc. (volumetric-based terms)
- Iterates over locally-owned edges for Advection/Diffusion terms (surface-based terms)



$$\int w S^\phi dV \approx \sum_{nd} S_{nd}^\phi V_{nd}$$

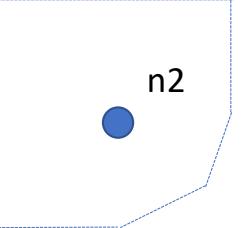
$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$$



EBVC: Implicit Time Discretization

- Let us define a general implicit time integrator that is A-stable
 - For $y' = k y ; y(0) = 1; y(t) = e^{kt}$ solution approaches zero as time increases for $k < 0$
- Backward Euler (two state) and is first-order accurate (A-stable)
- BDF2 (three state) is second-order accurate (A-stable)

This term is assembled over a nodal iteration and uses a single integration point (known as mass-lumping)


$$\int w \frac{\partial \rho \phi}{\partial t} dV \approx \sum_{nd} \frac{(\gamma_1 \rho_{nd}^{n+1} \phi_{nd}^{n+1} + \gamma_2 \rho_{nd}^n \phi_{nd}^n + \gamma_3 \rho_{nd}^{n-1} \phi_{nd}^{n-1})}{\Delta t} V_{nd}$$

For uniform time stepping, the coefficients are give by, $\gamma_1 = 3/2$ $\gamma_2 = -2$ $\gamma_3 = 1/2$



EBVC: Implicit Time Discretization; Code

- <https://github.com/NaluCFD/Nalu/blob/master/src/ScalarMassBDF2NodeSuppAlg.C>

```
//-----
//----- node_execute -----
//-----
void
ScalarMassBDF2NodeSuppAlg::node_execute(
    double *lhs,
    double *rhs,
    stk::mesh::Entity node)
{
    // deal with lumped mass matrix
    const double qNm1      = *stk::mesh::field_data(*scalarQNm1_, node);
    const double qN          = *stk::mesh::field_data(*scalarQN_, node);
    const double qNp1        = *stk::mesh::field_data(*scalarQNp1_, node);
    const double rhoNm1     = *stk::mesh::field_data(*densityNm1_, node);
    const double rhoN        = *stk::mesh::field_data(*densityN_, node);
    const double rhoNp1      = *stk::mesh::field_data(*densityNp1_, node);
    const double dualVolume = *stk::mesh::field_data(*dualNodalVolume_, node);
    const double lhsTime     = gamma1_*rhoNp1*dualVolume/dt_;
    rhs[0] -= (gamma1_*rhoNp1*qNp1 + gamma2_*qN*rhoN + gamma3_*qNm1*rhoNm1)*dualVolume/dt_;
    lhs[0] += lhsTime;
}
```

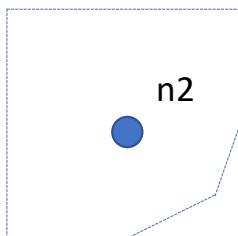


EBVC: Source Term Discretization

- Source terms for the edge-based scheme are also assembled over a nodal loop
- Note that in this scheme, we are using single point quadrature, i.e., the function is evaluated at a single point

The single point integration point leverages the fact that: $p = 2N - 1$

- Where N is the number of integration points and p is the polynomial order
- For a linear basis, using one-point quadrature is design-order, or second-order in space



$$\int w S^\phi dV \approx \sum_{nd} S_{nd}^\phi V_{nd}$$



EBVC: Source Term Discretization; Code

- https://github.com/NaluCFD/Nalu/blob/master/src/user_functions/VariableDensityMixFracSrcNodeSuppAlg.C

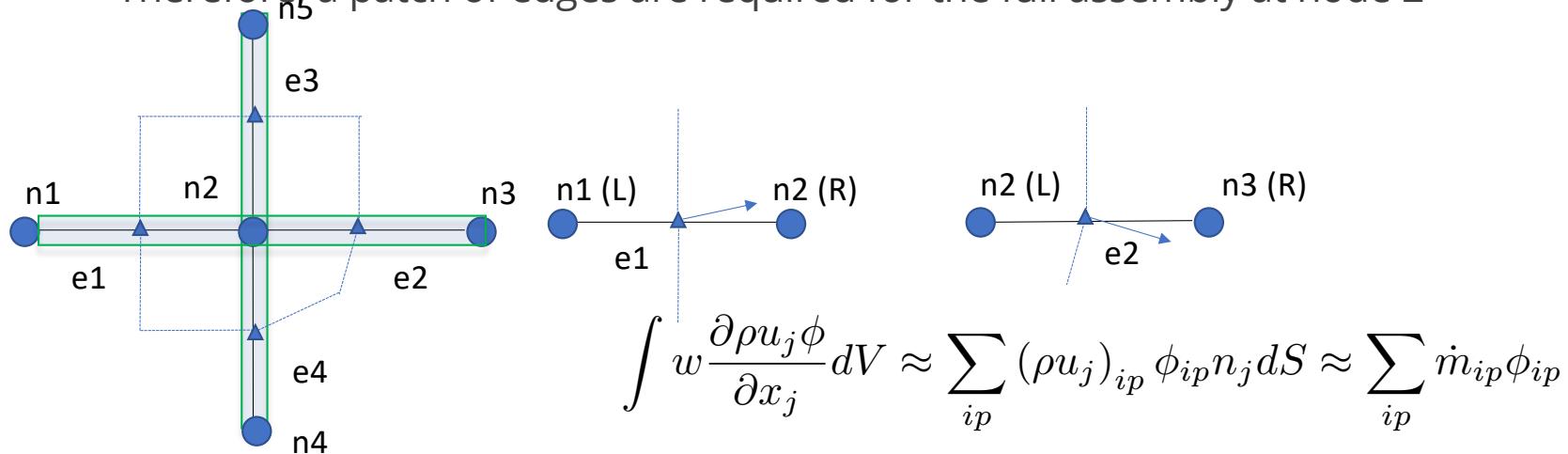
```
//-----
//----- node_execute -----
//-----
void
VariableDensityMixFracSrcNodeSuppAlg::node_execute(
    double /*lhs*/,
    double *rhs,
    stk::mesh::Entity node)
{
    // deal with lumped mass matrix
    const double *coords = stk::mesh::field_data(*coordinates_, node);
    const double dualVolume = *stk::mesh::field_data(*dualNodalVolume_, node );
    const double x = coords[0];
    const double y = coords[1];
    const double z = coords[2];

    const double src = 0.10e1 * pow(znot_ * cos(amf_ * pi_ * x) * cos(amf_ * pi_ * y) * cos(amf_
        rhs[0] += src*dualVolume;
}
```



EBVC: Advection Term Discretization

- For advection, we have transformed the volume integral to a surface integration
- Therefore, a patch of edges are required for the full assembly at node 2



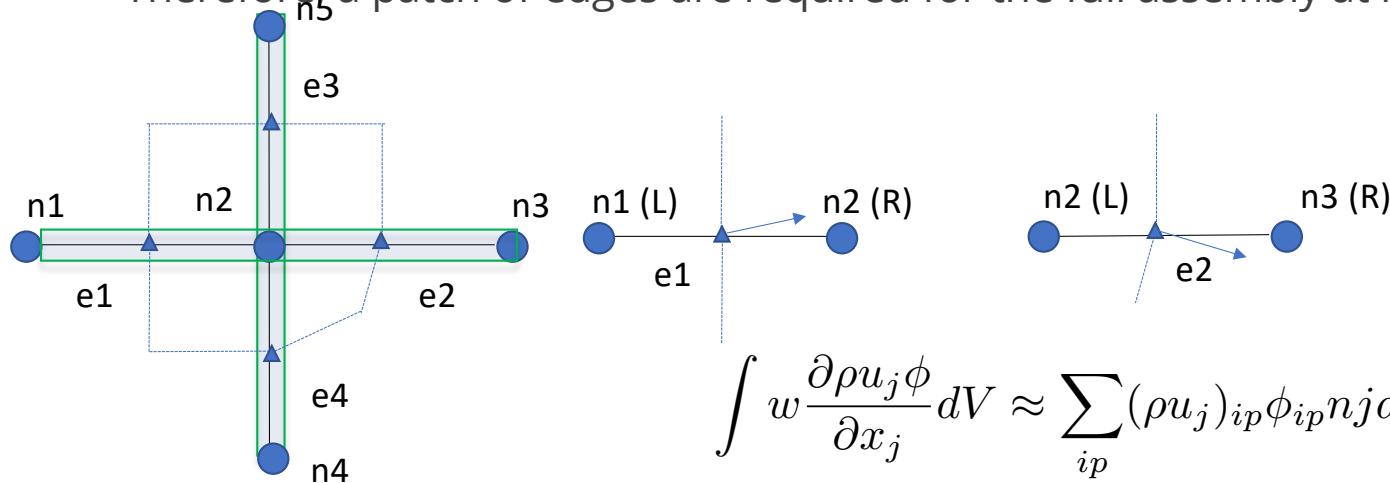
- Recall, that the mass flow rate at an integration point is prescribed
- Moreover, since the integration point is at the edge mid-point, $\phi_{ip} = (\phi^R + \phi^L)/2$

This is a *central-* or *Galerkin-based* advection operator; shown in conservative form, i.e, is in divergence form and has been integrated-by-parts



EBVC: Advection Term Discretization

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$$\int w \frac{\partial \rho u_j \phi}{\partial x_j} dV \approx \sum_{ip} (\rho u_j)_{ip} \phi_{ip} n_j dS \approx \sum_{ip} \dot{m}_{ip} \phi_{ip}$$

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This is a *central-* or *Galerkin-based* advection operator; shown in conservative form, i.e, is in divergence form and has been integrated-by-parts

Mahesh et al., JCP (2004)

For kinetic energy conservation, a CC scheme also uses $\frac{1}{2}$ weights!



EBVC: Advection Term Discretization; Code

- <https://github.com/NaluCFD/Nalu/blob/master/src/AssembleScalarEdgeSolverAlgorithm.C>



Upwind Advection Operators

- Recall from our finite difference class that in absence of a stabilizing diffusion term, or when the velocity is very high, i.e., the Peclet number > 2, non-physical oscillations can be noted
- An upwind approach was devised to mitigate this at the expense of numerical accuracy
- For a finite volume approach, upwinding is very easy to construct



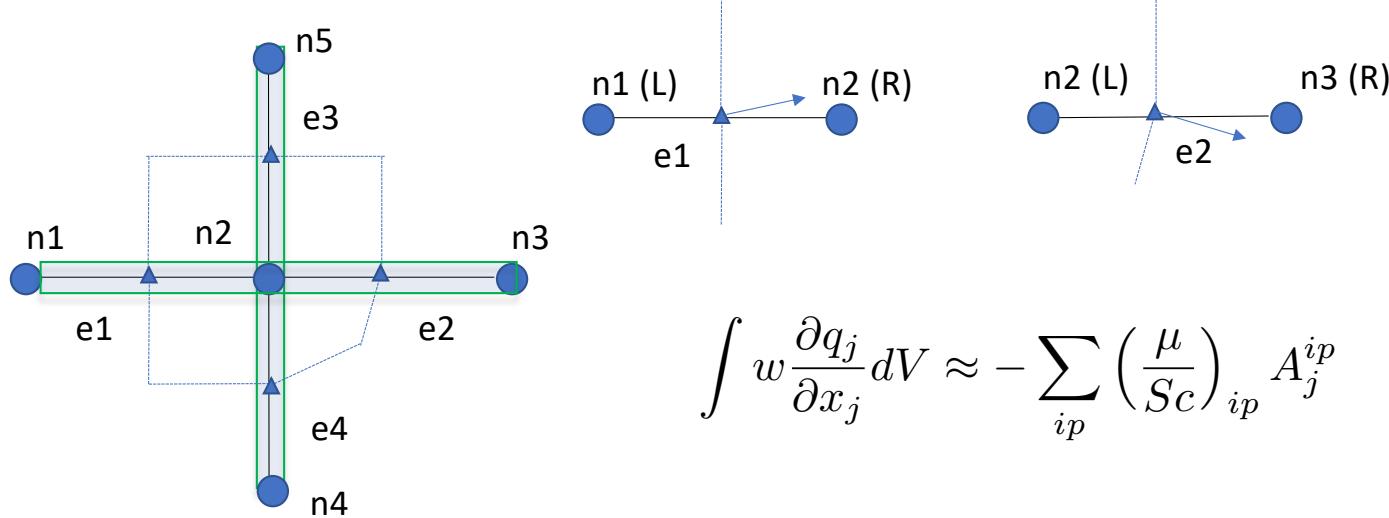
$$\phi_{j+1/2} = \begin{cases} \phi_j, & \text{if } u_l n_l > 0. \\ \phi_{j+1}, & \text{otherwise.} \end{cases} \quad \text{"as the wind blows"}$$

- However, upwind operators, even if higher-order, are numerically dissipative due to loss of symmetry of the operator
- Higher-order upwind (second-order in space) can be obtained on an unstructured mesh by use of projected nodal gradients and extrapolation (will cover this in the advection operator section)



EBVC: Diffusion

- For diffusion, we have transformed the volume integral to a surface integration
- Therefore, a patch of edges are required for the full assembly at node 2

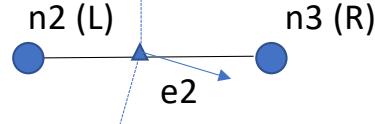




EBVC: Diffusion, Non-Orthogonality

- The edge-based diffusion operator is a bit more complex in that we are computing a gradient at the integration point while using two nodes, the left and right
- In many practical meshes, the distance vector between the edges (\mathbf{dx}_j) and the edge area vector will not be perfectly orthogonal
- This non-orthogonality causes inaccuracy when using a simplified approach

$$\frac{\partial \phi}{\partial x_j} = \frac{(\phi_R - \phi_L)}{|\Delta x_l|} n_j$$



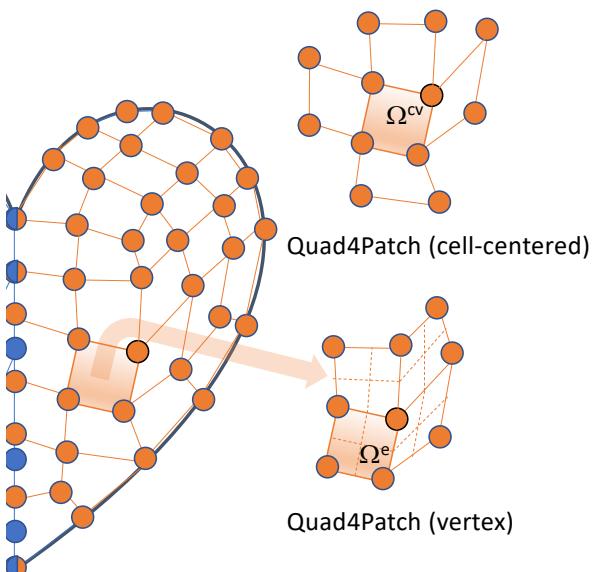
- The non-orthogonality approach of Jasek (Ph.D. Imperial College) is a standard cell-centered approach that has been adopted for edge-based schemes
- CC and EBVC are each two-state schemes and share non-orthogonality issues

$$\left. \frac{\partial \phi}{\partial x_j} \right|_{ip} = \overline{G_j \phi} + [(\phi_R - \phi_L) - \overline{G_l \phi} \Delta x_l] \frac{A_j}{A_k \Delta x_k}$$

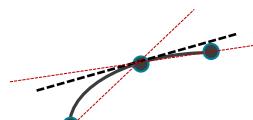
Where $G_j \phi$ is a “projected nodal gradient”

(Projected) Nodal Gradient Operator

- Recall, that the edge-based diffusion operator, and as we will see in future lectures for some choices for the advection operator, a nodal gradient is required



- First, the gradient of a function (other than linear) is discontinuous, i.e., the value at a shared element face depends on which element is used to compute the gradient
- Therefore, we can view the nodal gradient a continuous at the nodes and discontinuous within the elements



Let's minimize this difference: $\frac{1}{2} \left(\frac{\partial \phi}{\partial x_j} - G_j \phi \right)^2$
by solving:

$$\int w G_j \phi dV = \int w \frac{\partial \phi}{\partial x_j} dV \longrightarrow G_j \phi = \frac{\sum_{ip} \phi_{ip} n_j dS}{V}$$



EBVC: Diffusion, Non-Orthogonality; Code

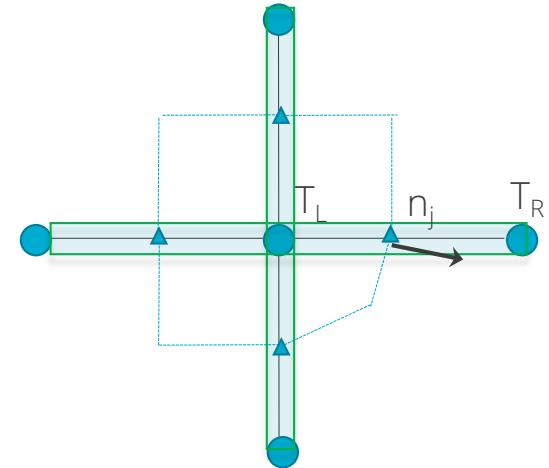
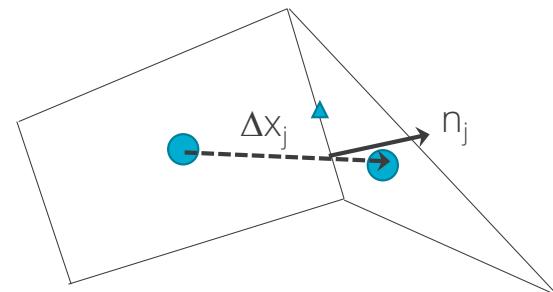
- <https://github.com/NaluCFD/Nalu/blob/master/src/AssembleScalarEdgeDiffSolverAlgorithm.C>

$$-\int w \frac{\mu}{Sc} \frac{\partial \phi}{\partial x_j} dV \approx - \left. \frac{\mu}{Sc} \right|_{ip} \left[(\overline{G_x \phi} A_x + \overline{G_y \phi} A_y) + (\phi_R - \phi_L) \frac{A_x A_x + A_y A_y}{A_x \Delta x_x + A_y \Delta x_y} - (\overline{G_x \phi} dx + \overline{G_y \phi} dy) \frac{A_x A_x + A_y A_y}{A_x dx + A_y dy} \right]$$



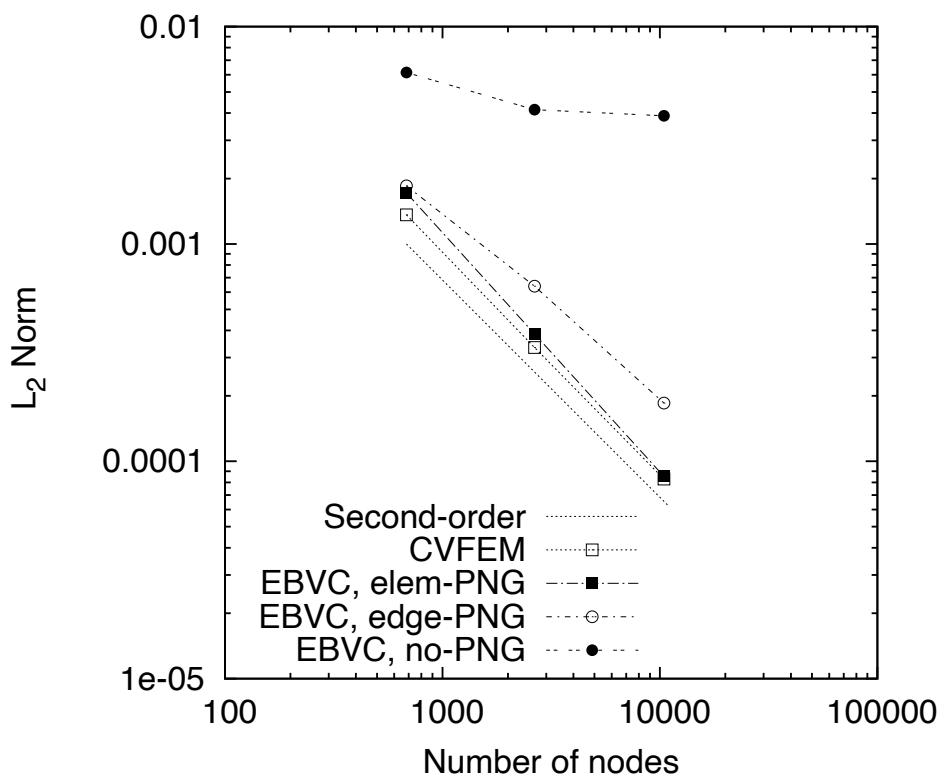
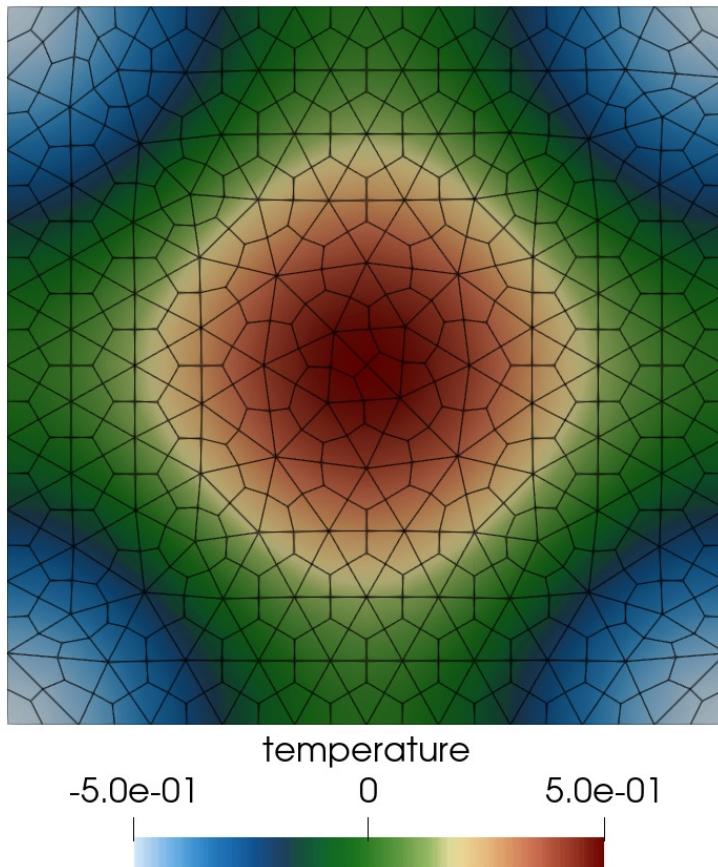
Typical Difficulties for a Two-State Scheme

- With two points, only a linear basis can be used, therefore, unstructured CC and EBVC are limited to second-order spatial accuracy
- Non-orthogonality, or the mis-alignment of the distance vector between the two "L" and "R" states and the surface normal, is present
- Integration point
- Both edge- and cell centered-based schemes show degraded accuracy on typical production meshes
- Several non-orthogonality approaches are available, for the best source, see Jasak
 - Jasak, "Error analysis and error estimation for the finite volume method with applications to fluid flow", Imperial College Dissertation, 1996





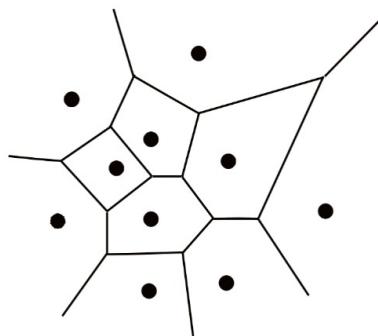
For Instance, Verification of The Diffusion Operator



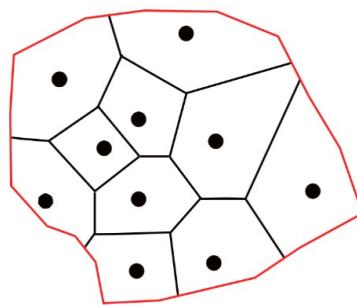


Arbitrary Polyhedra

- Thus far, we have described the element types as rather simple, e.g., Hex, Tet, Pyramid, and Wedge (or Prism)
- What if the element type was arbitrary and designed to minimize non-orthogonality?
 - Bres et al., *"Large-eddy simulations of co-annular turbulent jet using a Voronoi-based mesh generation framework"*, 2018 AIAA/CEAS Aeroacoustics Conference
 - Two-state limited to second-order-in-space (extensions exist)



(a) 2D Voronoi diagram



(b) 2D clipped Voronoi diagram

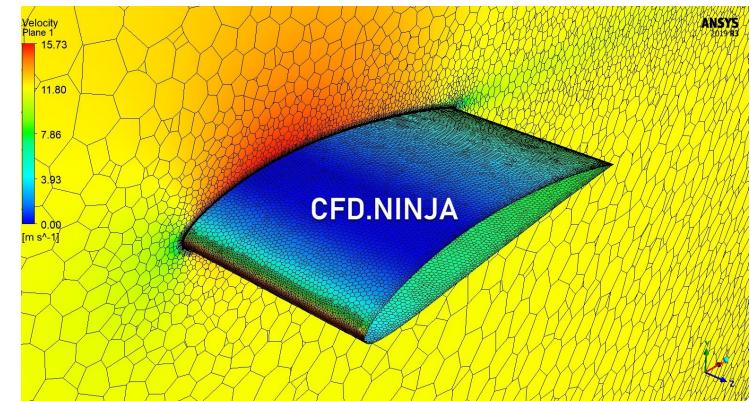


Figure 1. An arbitrary set of generating points (black circles) and the associated 2D Voronoi diagram (black lines). On the right a boundary surface (red lines) confines the mesh to a specific volume; note that the internal cell topology is unchanged.

Ansys-based arbitrary polyhedra
Exercised by <https://cfd.ninja>